

# Four-dimensional $CP^1 + U(1)$ lattice gauge theory for 3D antiferromagnets: Phase structure, gauge bosons and spin liquid

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In this paper we study the lattice  $CP^1$  model in  $(3+1)$  dimensions coupled with a dynamical compact  $U(1)$  gauge field. This model is an effective field theory of the  $s = \frac{1}{2}$  antiferromagnetic Heisenberg spin model in three spatial dimensions. By means of Monte Carlo simulations, we investigate its phase structure. There exist the Higgs, Coulomb and confinement phases, and the parameter regions of these phases are clarified. We also measure magnetization of  $O(3)$  spins, energy gap of spin excitations, and mass of gauge boson. Then we discuss the relationship between these three phases and magnetic properties of the high- $T_c$  cuprates, in particular the possibility of deconfined-spinon phase. Effect of dimer-like spin exchange coupling and ring-exchange coupling is also studied.

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The  $CP^N$  spin model plays an important role in various fields of physics not only as a tractable field-theory model that has interesting phase structure, but also as an effective field theory for certain systems in condensed matter physics and beyond. In particular, the  $CP^1$  model corresponds to the Schwinger-boson representation of the  $s = \frac{1}{2}$  antiferromagnetic (AF) quantum spin model, i.e., the AF Heisenberg model[1]. The  $CP^1$  model is much more tractable than the original AF Heisenberg model, and its phase structure and critical behavior have been investigated both analytically and numerically. The system intrinsically contains compact  $U(1)$  gauge degrees of freedom, and their dynamics determines the low-energy excitations in AF magnet. That is, if the gauge dynamics is in the deconfined-Coulomb phase, the low-energy excitations are the  $s = \frac{1}{2}$  spinons. On the other hand, the Higgs phase corresponds to the Néel state with a long-range AF order, and the confinement phase is a valence-bond solid (VBS) state in which spin-triplet low-energy excitations appear.

Most of the previous studies exploring a possible deconfined-spin-liquid phase have considered the two-dimensional (2D) (doped) AF Heisenberg model or its path-integral representation, the three-dimensional (3D)  $CP^1$  model. In these cases, the Coulomb phase may be possible if there exist sufficient number of gapless matter fields that couple to the gauge field. In fact, the problem whether deconfinement in a 3D  $U(1)$  gauge theory is possible was once a matter of controversy, but it seems now settled down, i.e., when the density of gapless excitations in matter sector is sufficiently large, the deconfinement phase takes place as a result of shielding mechanism[2].

In the present paper, we shall consider a higher-dimensional version of the 3D  $CP^1$  model, i.e., the 4D  $CP^1$  model coupled with a dynamical  $U(1)$  gauge field. This 4D  $CP^1 + U(1)$  gauge model is viewed as an effective field theory of the 3D AF Heisenberg model. From the gauge-theoretical point of view, the deconfinement na-

ture is *enhanced* in  $(3+1)$  D case because the Coulomb phase exists even in the pure 4D  $U(1)$  gauge system that involves no matter fields in contrast to the pure 3D  $U(1)$  gauge system that has only confinement phase. Therefore, it is interesting to study the phase structure of this 4D  $CP^1$  gauge model. We shall first consider the  $CP^1$  model for the 3D AF Heisenberg model with uniform nearest-neighbor spin coupling and then the  $CP^1$  model for the 3D AF Heisenberg model with nonuniform dimer-like coupling and ring-exchange spin coupling.

The  $CP^1$  variable  $z_x$  is put on the site  $x$  of the 4D hypercubic (space-imaginary time) lattice.  $z_x$  is a two-component complex field satisfying the  $CP^1$  constraint,  $z_x \equiv (z_{x1}, z_{x2})^t$ ,  $\sum_{a=1}^2 |z_{xa}|^2 = 1$ . In path-integral, the  $s = \frac{1}{2}$  spin operator  $\hat{S}_r$  at the spatial site  $r$  is mapped to a classical  $O(3)$  spin  $\vec{S}_x = \vec{z}_x \vec{\sigma} z_x$  satisfying  $\vec{S}_x \cdot \vec{S}_x = 1$  where  $x = (r, x_0)$  and  $\vec{\sigma}$  are the Pauli spin matrices. The  $U(1)$  gauge field  $U_{x\mu} \equiv \exp(i\theta_{x\mu})$  ( $\mu = 1, \dots, 4$  is the direction index and denotes also the unit vector in the  $\mu$ -th direction) is put on the link  $(x, \mu)$  connecting sites  $x$  and  $x + \mu$ .

The  $CP^1$  field theory in the continuum is derived from the 3D AF Heisenberg model by integrating out the half of the  $CP^1$  variables (on all the odd sites) by assuming a short-range AF order[1]. In order to study the model numerically, we reformulate the model by putting it on the 4D hypercubic lattice, which has the correct continuum limit. Then the action  $S$  of the  $CP^1$  model is given as

$$S = -\frac{c_1}{2} \sum_{x, \mu, a} \left( \bar{z}_{x+\mu, a} U_{x\mu} z_{xa} + \text{H.c.} \right) - \frac{c_2}{2} \sum_{x, \mu < \nu} \left( \bar{U}_{x\nu} \bar{U}_{x+\nu, \mu} U_{x+\mu, \nu} U_{x\mu} + \text{H.c.} \right), \quad (1)$$

where  $c_1$  and  $c_2$  are parameters of the model.

Qualitative estimation of the parameters in the action (1) is obtained as follows. By choosing the lattice spacing

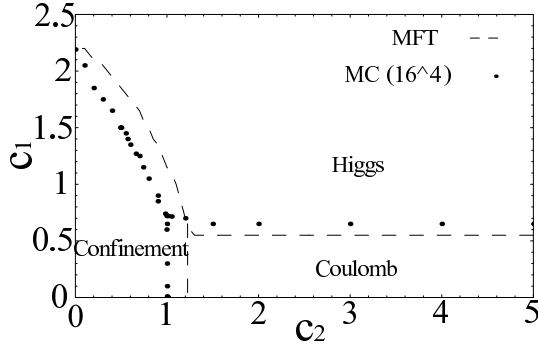


FIG. 1: Phase diagram of the 4D  $CP^1$  model (1) in the  $c_2 - c_1$  plane obtained by Monte Carlo simulation (circles) and by mean field theory (dashed curves). The Higgs-Coulomb and confinement-Coulomb phase transitions are of second order, whereas the Higgs-confinement transition is of first-order in the region near the tricritical point, and becomes second-order for higher  $c_1$ . For example,  $(c_2, c_1) = (0.96, 1.27)$  is of first order and  $(0.87, 1.40)$  is of second order.

in the time direction  $a_0$  suitably, we obtain Eq.(1) with  $c_1$  a *constant* independent of the exchange coupling  $J$  of the AF Heisenberg model, and  $c_2 = 0$ [3]. However, via the renormalization effect of high-momentum modes of spinons  $z_x$ , not only the  $c_1$ -term is renormalized but also the  $c_2$ -term is generated.

When holes are doped into an AF magnet like the high- $T_c$  cuprate at half-filling, the system is described by a canonical model like the t-J model. The t-J model can be studied by the slave-fermion- $CP^1$  representation[1]. One can see that as a result of the hole doping in the short-range AF background, the parameter  $c_1$  is renormalized. If the hopping of holons is ignored,  $c_1 \rightarrow (1 - \delta)c_1$  where  $\delta$  is the hole concentration. Furthermore, the short-range AF order generates attractive force between holes sitting on nearest-neighbor sites, and it indicates the appearance of the superconducting phase. When the hole-pair field  $M_{x,i}$  ( $i = 1, 2, 3$ : spatial direction index) condenses, the  $c_2$ -plaquette term in Eq.(1) is generated by the hopping of quasiparticles (i.e., the gapped holons)[1].

The phase diagram of the model (1) in the  $c_2 - c_1$  plane has been determined by calculating the “internal energy” per site  $E = \langle S \rangle / V$  and the “specific heat” per site  $C = \langle (S - E)^2 \rangle / V$  by means of Monte Carlo simulations for a lattice of size  $V = L^4$  with the periodic boundary condition in the previous paper[4]. We show the result in Fig.1. In Fig.1, we also show the result obtained by the mean-field approximation. There are three phases in the  $c_2 - c_1$  plane. We expect and verify that these three phases are *Higgs*, *confinement* and *Coulomb* phases in the gauge-theory terminology, respectively. The Higgs phase is nothing but the Néel state of the AF magnets. There deconfined gapless spinons are spin-wave magnons. The confinement phase is a spin-liquid phase in which the low-energy excitations are *spin-triplet bound states* of  $z_x$ . On the other hand, the Coulomb phase corresponds to a *deconfined spin liquid* in which the low-energy excitations

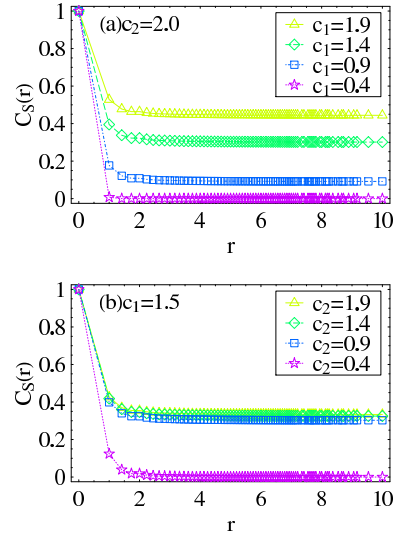


FIG. 2: Spin-spin correlation functions  $C_S(r)$  for  $12^4$  lattice. (a)  $c_2 = 2.0$ ; (b)  $c_1 = 1.5$ . The magnetization is finite in the Higgs phase.

are  $s = \frac{1}{2}$  spinons  $z_x$  with a gap. We shall see that the gauge-boson mass vanishes in the Coulomb phase while it remains finite in the other two phases.

In Ref.[5] we have studied the phase structure of the  $CP^1 + U(1)$  model (1) not on the 4D lattice but on the *3D lattice*. We found that the Coulomb phase is missing. The gauge-boson mass takes its minimum value just on the critical line separating the Higgs and confinement phases. If we include  $N_f$ -fold  $CP^1$  variables, the gauge-boson mass on the critical line vanishes for  $N_f \geq 14$ [6]. The original uniform AF Heisenberg model is in the Néel state, which corresponds to the Higgs phase[1].

In Fig.2, we show the result of our calculations of the  $O(3)$  spin-spin correlation functions,  $C_S(r) = \langle \vec{S}_{x+r} \cdot \vec{S}_x \rangle$ . From Fig.2 we see that the spontaneous magnetization,  $[C_S(r_{\max})]^{1/2}$  ( $r_{\max} \equiv L$ ), is nonvanishing only in the Higgs phase as expected.

In Fig.3 we show the mass gap  $M_S$  of the spin excitations that is obtained from  $C_S(r) - C_S(r_{\max})$ . Fig.3 shows that  $M_S$  is vanishing in the Higgs phase as expected.

Next, we study the dynamics of gauge bosons by mea-

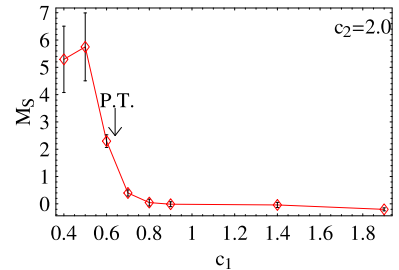


FIG. 3: Mass  $M_S$  of spin excitations for  $c_2 = 2.0$ . P.T. indicates the location of transition point in Fig.1.  $M_S$  vanishes in the Néel state (Higgs phase).

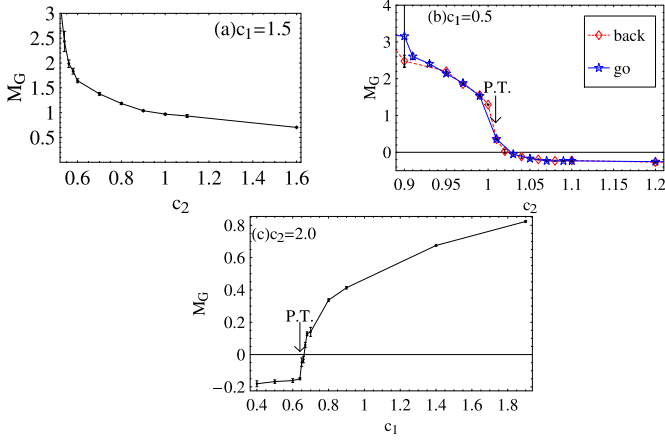


FIG. 4: Gauge-boson mass  $M_G$  of (4). (a)  $c_1 = 1.5$  (b)  $c_1 = 0.5$  (c)  $c_2 = 2.0$ .  $M_G$  vanishes only in the Coulomb phase. (Negative value of  $M_G$  is a finite-size effect. See Ref.[6].)

asuring the gauge-boson mass  $M_G$ , which is calculated from the correlation function of gauge flux,

$$O_{\mu\nu}(x) = \sum_{\lambda, \eta} \epsilon_{\mu\nu\lambda\eta} \text{Im} \bar{U}_{x\lambda} \bar{U}_{x+\lambda, \eta} U_{x+\eta, \lambda} U_{x\eta}, \quad (2)$$

where  $\epsilon_{\mu\nu\lambda\eta}$  is the totally antisymmetric tensor. To estimate  $M_G$  precisely, we introduced the Fourier-transform  $\tilde{O}$  and measured its correlation,

$$\tilde{O}(x_\mu, x_\nu) = \sum_{x_\lambda, x_\eta} O_{\mu\nu}(x) e^{ip_\lambda x_\lambda + ip_\eta x_\eta},$$

$$D_G(y_\mu, y_\nu) = \frac{1}{L^4} \sum_{x_\mu, x_\nu} \langle \tilde{O}(x_\mu, x_\nu) \tilde{O}(x_\mu + y_\mu, x_\nu + y_\nu) \rangle, \quad (3)$$

with setting  $p_\lambda = p_\eta = 1/L$  where  $L$  is the system size. We fit the data in the following form[7];

$$D_G(y_\mu, y_\nu) \propto \exp \left( -\sqrt{p_\mu^2 + p_\nu^2 + M_G^2} \sqrt{y_\mu^2 + y_\nu^2} \right). \quad (4)$$

In Fig.4, we show  $M_G$ . We can see that  $M_G$  is vanishing in the Coulomb phase as it should be, whereas it is finite in the other phases.

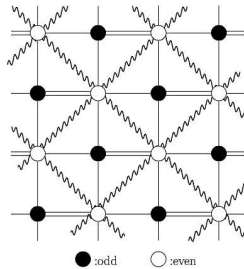


FIG. 5: AF Heisenberg model with dimer and ring couplings. The double-line bonds have larger exchange than that of the single-line bond. The wavy lines represent ring coupling among four spins on each square of even-sites.

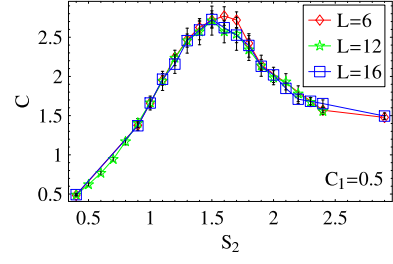


FIG. 6: Specific heat of the 3D plaquette model (5) for  $c_1 = 0.5$  as a function of  $s_2$ . There is no system-size dependence in  $C$ , indicating a crossover near the round peak.

The above measurements confirm the phase structure of the model (1) given in Fig.1. From this result, we can discuss how the magnetic properties of the doped AF magnets with strong three-dimensionality changes under doping at zero temperature. Undoped and lightly doped uniform AF magnets in 3D has the Néel order and is in the Higgs phase. As  $\delta$  is increases, the system loses the Néel order and enters the confinement or Coulomb phase depending on the mobility of doped holes. In the framework of the t-J model, this problem is under study and the result will be published in near future[8].

In the rest of this paper, we shall consider the  $CP^1$  gauge model with the 3D spatial gauge-plaquette term. The action  $S'$  of this 3D plaquette model is given by

$$S' = -\frac{c_1}{2} \sum_{x, \mu, a} \left( \bar{z}_{x+\mu, a} U_{x\mu} z_{xa} + \text{H.c.} \right) - \frac{s_2}{2} \sum_{x, i, j=1}^3 (i < j) \left( \bar{U}_{xj} \bar{U}_{x+j, i} U_{x+i, j} U_{xi} + \text{H.c.} \right) \quad (5)$$

In contrast to the  $c_2$  term of the 4D plaquette model (1), the  $s_2$ -term in Eq.(5) contains only the *spatial-plaquette* terms and no space-time plaquette terms. The 3D plaquette model (5) is an effective low-energy model of *nonuniform* AF Heisenberg model with dimer-like couplings and ring-exchange couplings. The parameter  $c_1$  decreases as the dimer coupling increases[9] and the  $s_2$  term corresponds to ring coupling like  $(\vec{S}_i \cdot \vec{S}_j)(\vec{S}_k \cdot \vec{S}_l)$  where  $(i, j, k, l)$  denote even sites forming a square in even sublattice. (See Fig.5.) Thus the bare value of  $s_2$  is finite in contrast to the 4D plaquette model (1) for the sym-

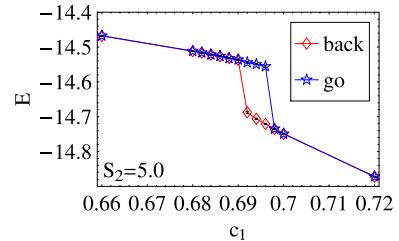


FIG. 7: Internal energy of the 3D plaquette model (5) for  $s_2 = 5.0$ . It shows a hysteresis curve.

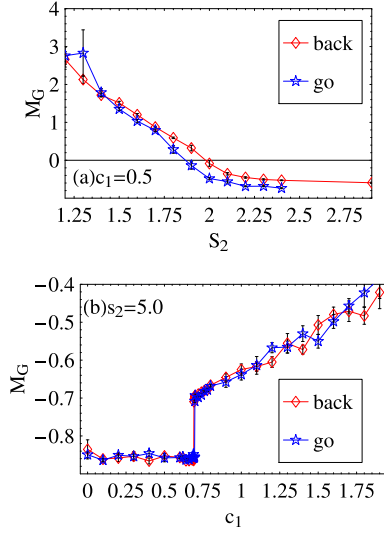


FIG. 8: Gauge boson mass  $M_G$  in the model (5). (a)  $c_1 = 0.5$ ; (b)  $s_2 = 5.0$ [10].

metric Heisenberg model where the bare value of  $c_2 = 0$ .

It is interesting to see if the Coulomb phase (deconfined spin-liquid phase), which exists in the model (1), survives in the present model. Therefore we investigated the phase structure of the model (5) first by calculating the internal energy and the specific heat. Some of our results are shown in Figs.6 and 7. From these calculations, we conclude that the model  $S'$  of (5) has similar phase structure to that of  $S$  of (1). But the second-order

confinement-Coulomb phase transition in the model  $S$  becomes a *crossover* in  $S'$  as Fig.6 shows, i.e., the specific heat has a rather smooth peak that has *no system-size dependence*. We think that this crossover is similar to that in the 3D Abelian gauge-Higgs model. Furthermore, the phase transitions at  $c_1 \simeq 0.7$  in the region of  $s_2 \gtrsim 1.5$  are of *first order* as indicated in Fig.7.

In order to verify the above conclusion, we calculated  $M_G$ , which is shown in Fig.8. It is obvious that along with  $c_1 = 0.5$   $M_G$  decreases smoothly as  $s_2$  is increased crossing the crossover line at  $s_2 \simeq 1.5$ . This behavior is very close to that in the Abelian gauge-Higgs system observed in Ref.[6]. On the other hand, along the line  $s_2 = 5.0$   $M_G$  exhibits a sharp discontinuity. Its behavior verifies the first-order phase transition at  $c_1 \simeq 0.7$ [10].

Then we draw the following conclusions;

1. In contrast to the 4D plaquette model  $S$ , the 3D plaquette model  $S'$  does not support the Coulomb phase, i.e., the deconfined spin-liquid phase is not realized in the nonuniform AF Heisenberg model[11, 12].
2. The Néel-VBS phase transition caused by the ring-exchange coupling is of first-order. Recent numerical study on some related AF Heisenberg models gives similar conclusion[12].

In summary, we studied the 4D  $CP^1$  model coupled with 4D or 3D  $U(1)$  gauge field and revealed its phase structure. We discussed some physical implications for various 3D AF Heisenberg magnets, i.e., with and without doping and with uniform or nonuniform coupling in gauge-theoretical viewpoints.

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  - [10] Negative values of  $M_G$  in Fig.8 come from the definition of  $M_G$ . The plaquette term with fairly large coefficient ( $s_2 = 5.0$ ) severely suppresses fluctuations of the gauge field in the present case.
  - [11] Nonetheless, for the Abelian gauge-Higgs model in 3D, it was suggested that the across the crossover line certain nonlocal physical quantities like flux-line density exhibit typical behavior of second-order phase transition. See S.Wenzel, E.Bittner, W.Janke, and A.M.J.Schakel, arXiv:0708.0903. We expect similar behavior for the present model  $S'$ .
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